

Ecotox Report for Case # P-18-0077

General

| | |
|--|---|
| Status 09/19/2018 Date: SAT Date: 01/05/2018 | Report Status: Complete CRSS Date: 01/04/2018 SAT T. Chair: Behrsing |
| Consolidated N PMN: Ecotox Analogs: [REDACTED] | Consolidated Set: |
| Related Cases: [REDACTED] | |
| Health Related ANALOGS: Cases: [REDACTED] | |
| Submitter: Koch Agronomic Services | |
| CAS Number: 2093385-47-6 | |
| Chemical Urea, Name: reaction products with N-butylphosphorothioic triamide and formaldehyde | |
| Use: Reagent for the controlled release of a urease inhibitor in urea-based fertilizers used on farms. %Phosphorus = 12.4% (measured). P2REC: CRSS: Forward. P2 Claim: The PMN material is intended to replace direct use of N-butyl-phosphorothioic triamide [REDACTED] in fertilizer formulations. NBPT, when in contact with the soil, degrades in a relatively short period of time through oxidation and hydrolysis. The PMN material is stable enough to extend the availability of NBPT, while being labile enough that NBPT is released when water is present, ensuring that a low level of NBPT is present for the days or weeks during which the urea fertilizer is taken up by the crop. | |
| Trade Name: Anvol (TM)-trademarked name of the final product formulation | |
| PV-max(kg/yr): [REDACTED] | Ecotox Assessor: Kennedy, Amuel |

Fate Summary Statement

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| Fate P-18-0077 Summary Statement: FATE: Estimations for hydrolysis product N-butylphosphorothioic triamide, MW = 167, C ₄ H ₁₄ N ₃ PS log Kow = 0.44 (M) |
|--|

log Koc =

1.34 (E)

log Fish BCF = 0.50 (3) (E)

log Fish BAF = 0.03 (1) (E)

FATE: Estimations for hydrolysis product urea-formaldehyde oligomer, MW = 162, C₄H₁₀N₄O₃

log Kow = -4.01 (E)

log Koc = 1.00 (E)

log

Fish BCF = 0.50 (3) (E)

log Fish BAF = -0.05 (1) (E)

PMN

Substance: Solid with MP = Dec. 150 °C (M)

log Kow = 0.60 (M for mixture)

S = Reacts / 35 mg/L at 25 °C / 37 g/L at 25 °C (M / M for mixture / E)

Hydrolysis Half-life = hr-da

VP = 3.3E-6 torr at 25

°C (E)

BP = 393 °C (E)

H < 1.00E-8 (E)

POTW removal (%) =

PMN 90 via hydrolysis; then Hyd Pdt NBPT 0-10;

Hyd Pdt

urea-formaldehyde oligomers 75-90 via biodeg and hydrolysis; Hydrolysis (OPPTS 835.2120): t_{1/2}(pH4,7,9):hr/hr-da/da

Time for complete ultimate

aerobic biodeg = Hyd Pdt NBPT > mo;

Hyd Pdt urea-formaldehyde oligomers wk

Sorption to soils/sediments = Hyd Pdt NBPT low; Hyd Pdt urea-formaldehyde oligomers low

PBT Potential: PMN P1B1; Hyd Pdt NBPT

P3B1; Hyd Pdt urea-formaldehyde oligomers P1B1

*CEB FATE: Migration to

ground water = Hyd Pdt NBPT rapid;

Hyd Pdt urea-formaldehyde oligomers slow

Bioconcentration factor to be put into E-FAST: Hyd Pdt NBPT 3;

Hyd Pdt urea-formaldehyde oligomers 3

PMN Material:

Overall wastewater treatment removal is 90% via rapid hydrolysis (hydrolysis half-life: hours to days).

PMN Material:

Low

Persistence (P1) is based on rapid hydrolysis (hydrolysis half-life: hours to days).

Low Bioaccumulation potential (B1) is based on rapid hydrolysis (hydrolysis half-life: hours to days).

Hydrolysis Product

(N-butylphosphorothioic triamide):

Overall wastewater treatment

removal is 0-10% via low biodegradability, low sorption and low stripping.

Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.

Air Stripping

(Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.

Removal by biodegradation in wastewater treatment is negligible based on BIOWIN model estimates and data from analogous chemicals.

The

aerobic aquatic biodegradation half-life is greater than months based on BIOWIN model estimates and data from analogous chemicals.

The

anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Hydrolysis half-life is greater than

months based on measured data (hydrolysis half-life: 92 days at pH 7 and 58 minutes at pH 3).

Sorption to soil and sediment is low based on

the estimated physical-chemical properties from EPISUITE.

Migration

to groundwater is rapid based on the estimated physical-chemical properties from EPISUITE.

Hydrolysis Product (N-butylphosphorothioic triamide):

High Persistence (P3) is based on the estimated anaerobic biodegradation half-life.

Low Bioaccumulation potential (B1) is based on the BCFBAF model estimates.

Hydrolysis Product

(Urea-Formaldehyde oligomer):

Overall wastewater treatment removal is 75-90% via biodegradation and hydrolysis.
 Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.
 Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.
 Removal by biodegradation in wastewater treatment is moderate based on BIOWIN model estimates.

The aerobic aquatic biodegradation half-life is weeks based on BIOWIN model estimates.

The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Hydrolysis half-life is days based on analogous chemicals and professional judgment.

Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE.

Migration to groundwater is slow, mitigated by biodegradation and hydrolysis.

Hydrolysis

Product (Urea-Formaldehyde oligomer):

Low Persistence (P1) is based on further hydrolysis of the urea-formaldehyde oligomer (hydrolysis half-life: days).

Low Bioaccumulation potential (B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast: 3 (hydrolysis products).

Physical Chemical Information

| | | |
|-------------------------------|--------|--|
| Molecular Weight: | 239.23 | |
| Wt% < 500: | | Wt% < 1000: |
| Physical State - Neat: | Solid | |
| Melting Point: | | Melting Point (est): Dec. ca. 150 |
| MP (EPI): | 85.17 | |
| Vapor Pressure: | | Vapor Pressure (est): 0.000003 |

| | | | |
|-------------------------|-----------|--------------------------|-------------|
| VP | 3.29e-006 | | |
| (EPI): | | | |
| Water | 0.035000 | Water | 37.1/Reacts |
| Solubility: | | Solubility (est): | |
| Water Solubility | | | |
| (EPI): | | | |
| Henry's Law:: | | | |
| Log Koc: | | Log | |
| | | Koc (EPI): | |
| Log | | Log | -1.69 |
| Kow: | | Kow (EPI): | |
| Log | | | |
| Kow Comment: | | | |

SAT**Concern Level**

| | | | |
|------------------------|-----------------|--|--|
| Ecotox | 2 | | |
| Rating (1): | | | |
| Ecotox | | | |
| Rating Comment | | | |
| (1): | | | |
| Ecotox Rating | | | |
| (2): | | | |
| Ecotox | | | |
| Rating Comment | | | |
| (2): | | | |
| Ecotox Route of | All releases to | | |
| Exposure: | water | | |

Ecotox Comments

| | | | |
|-----------------------|---|--|--|
| Exposure | Y | | |
| Based Review | | | |
| (Eco): | | | |
| Ecotox | | | |
| Comments: | | | |
| Exposure Based | | | |
| Testing: | | | |

PBT Ratings

| Persistence | Bioaccumulation | Toxicity | Comments |
|--------------------|------------------------|-----------------|-----------------|
| 1 | 1 | 2 | PMN |
| 3 | 1 | 2 | Hyd |
| | | | Pdt |
| | | | NBPT |

| Persistence | Bioaccumulation | Toxicity | Comments |
|-------------|-----------------|----------|---|
| 1 | 1 | 2 | Hyd Pdt urea-formaldehyde oligomers |

Eco-Toxicity Comment:

Fate Ratings

| Removal90;0-10;75-90 in WWT/POTW (Overall): Condition | | | | | | |
|--|------|------------|----------|----------|--------------------|------------------------------|
| Rating Values | 1 | 2 | 3 | 4 | Rating Description | |
| | | | | | | Comment |
| Fish BCF: | | | | | | |
| Log Fish BCF: | | | | | | |
| WWT/POTW Sorption: | ;1;1 | Low | Moderate | Strong | V. Strong | |
| WWT/POTW Stripping: | ;4;4 | Extensive | Moderate | Low | Negligible | |
| Biodegradation Removal: | ;4;3 | Unknown | High | Moderate | Negligible | |
| Biodegradation Destruction: | | Unknown | Complete | Partial | — | |
| Aerobic Biodeg Ult: | ;4;2 | <= Days | Weeks | Months | > Months | |
| Aerobic Biodeg Prim: | | <= Days | Weeks | Months | > Months | |
| Anaerobic Biodeg Ult: | ;4;4 | <= Days | Weeks | Months | > Months | |
| Anaerobic Biodeg Prim: | | <= Days | Weeks | Months | > Months | |
| Hydrolysis (t1/2 at pH 7,25C) A: | | <= Minutes | Hours | Days | >= Months | P-NR |
| Hydrolysis (t1/2 at pH 7,25C) B: | | <= Minutes | Hours | Days | >= Months | |
| Sorption to Soils/Sediments: | ;4;4 | V. Strong | Strong | Moderate | Low | |
| Migration to Ground Water: | ;4;2 | Negligible | Slow | Moderate | Rapid | ;Hyd Pdt NBPT rapid; Hyd Pdt |

| Removal 90;0-10;75-90 in WWT/POTW (Overall): | | | | | |
|---|------------------|------------|------|-------------------------|--|
| Condition | Rating Values | 1 | 2 | Rating Description 3 | 4 |
| | | | | | urea- formaldehyde oligomers slow |
| Photolysis A, Direct: | | Negligible | Slow | Moderate | Rapid |
| Photolysis B, Indirect: | | Negligible | Slow | Moderate | Rapid |
| Atmospheric Ox A, OH: | | Negligible | Slow | Moderate | Rapid |
| Atmospheric Ox B, O3: | | Negligible | Slow | Moderate | Rapid |
| Bio Comments: PMN Material: Overall wastewater treatment removal is 90% via rapid hydrolysis (hydrolysis half-life: hours to days). PMN Material: Low Persistence (P1) is based on rapid hydrolysis (hydrolysis half-life: hours to days). Low Bioaccumulation potential (B1) is based on rapid hydrolysis (hydrolysis half-life: hours to days). Hydrolysis Product (N-butylphosphorothioic triamide): Overall wastewater treatment removal is 0-10% via low biodegradability, low sorption and low stripping. Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates. Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates. Removal by biodegradation in wastewater treatment is negligible based on BIOWIN model estimates and data from analogous chemicals. The aerobic aquatic biodegradation half-life is greater than months based on BIOWIN model estimates and data from analogous chemicals. The anaerobic aquatic biodegradation half-life is greater | | | | | |

| Removal 90;0-10;75-90 in WWT/POTW (Overall): | | | | | |
|--|---------------|---|---|--|-----------|
| Condition | Rating Values | 1 | 2 | Rating Description | 34Comment |
| | | | | than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life. Hydrolysis half-life is greater than months based on measured data (hydrolysis half-life: 92 days at pH 7 and 58 minutes at pH 3). Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE. Migration to groundwater is rapid based on the estimated physical-chemical properties from EPISUITE. Hydrolysis Product (N-butylphosphorothioic triamide): High Persistence (P3) is based on the estimated anaerobic biodegradation half-life. Low Bioaccumulation potential (B1) is based on the BCFBAF model estimates. Hydrolysis Product (Urea-Formaldehyde oligomer): Overall wastewater treatment removal is 75-90% via biodegradation and hydrolysis. Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates. Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates. Removal by biodegradation in wastewater treatment is moderate based on BIOWIN model estimates. The aerobic aquatic biodegradation half-life is weeks based on BIOWIN model estimates. The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life. Hydrolysis half-life is days based on analogous chemicals and professional judgment. Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE. | |

| | | | | |
|--|--|--|--|--|
| Removal 90;0-10;75-90 in WWT/POTW (Overall): Condition Rating Rating Description Comment Values 1 2 3 4 | | | | |
| <p>Migration to groundwater is slow, mitigated by biodegradation and hydrolysis.</p> <p>Hydrolysis Product (Urea-Formaldehyde oligomer):</p> <p>Low Persistence (P1) is based on further hydrolysis of the urea-formaldehyde oligomer (hydrolysis half-life: days).</p> <p>Low</p> <p>Bioaccumulation potential (B1) is based on BCFBAF model estimates.</p> <p>Bioconcentration/Bioaccumulation factor to be put into E-Fast: 3 (hydrolysis products).</p> <p>Fate PMN Material:</p> <p>Comments: Overall</p> <p>wastewater treatment removal is 90% via rapid hydrolysis (hydrolysis half-life: hours to days).</p> <p>PMN Material:</p> <p>Low Persistence (P1) is based on rapid hydrolysis (hydrolysis half-life: hours to days).</p> <p>Low</p> <p>Bioaccumulation potential (B1) is based on rapid hydrolysis (hydrolysis half-life: hours to days).</p> <p>Hydrolysis Product (N-butylphosphorothioic triamide):</p> <p>Overall wastewater treatment removal is 0-10% via low biodegradability, low sorption and low stripping.</p> <p>Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.</p> <p>Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.</p> <p>Removal by biodegradation in wastewater treatment is negligible based on BIOWIN model estimates and data from analogous chemicals.</p> <p>The aerobic aquatic biodegradation half-life is greater than months based on BIOWIN model estimates and data from analogous chemicals.</p> <p>The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation</p> | | | | |

| Removal 90;0-10;75-90 in WWT/POTW (Overall): | | | | | Comment |
|--|------------------|---|---|-------------------------|--|
| Condition | Rating Values | 1 | 2 | Rating Description 3 | |
| | | | | 4 | |
| | | | | | <p>half-life is projected to be greater than or equal to the aerobic biodegradation half-life.</p> <p>Hydrolysis half-life is greater than months based on measured data (hydrolysis half-life: 92 days at pH 7 and 58 minutes at pH 3).</p> <p>Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE.</p> <p>Migration to groundwater is rapid based on the estimated physical-chemical properties from EPISUITE.</p> <p>Hydrolysis Product (N-butylphosphorothioic triamide):</p> <p>High Persistence (P3) is based on the estimated anaerobic biodegradation half-life.</p> <p>Low Bioaccumulation potential (B1) is based on the BCFBAF model estimates.</p> <p>Hydrolysis Product (Urea-Formaldehyde oligomer):</p> <p>Overall wastewater treatment removal is 75-90% via biodegradation and hydrolysis.</p> <p>Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.</p> <p>Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.</p> <p>Removal by biodegradation in wastewater treatment is moderate based on BIOWIN model estimates.</p> <p>The aerobic aquatic biodegradation half-life is weeks based on BIOWIN model estimates.</p> <p>The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.</p> <p>Hydrolysis half-life is days based on analogous chemicals and professional judgment.</p> <p>Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE.</p> <p>Migration to groundwater</p> |

| Removal 90;0-10;75-90 in WWT/POTW (Overall): | | | | | |
|---|--------|---|--------------------|---|--|
| Condition | Rating | | Rating Description | | Comment |
| | Values | 1 | 2 | 3 | 4 |
| | | | | | <p>is slow, mitigated by biodegradation and hydrolysis.</p> <p>Hydrolysis</p> <p>Product (Urea-Formaldehyde oligomer):</p> <p>Low Persistence (P1) is based on further hydrolysis of the urea-formaldehyde oligomer (hydrolysis half-life: days).</p> <p>Low Bioaccumulation potential (B1) is based on BCFBAF model estimates.</p> <p>Bioconcentration/Bioaccumulation factor to be put into E-Fast: 3 (hydrolysis products).</p> |

Ecotoxicity Values

| Test organism | Test Type | Test Endpoint | Predicted | Experimental | Comments |
|---|-----------|---------------|-----------|--------------|---|
| Fish | 96-h | LC50 | >100 | 780 | Est Top Left; Anlg [REDACTED] |
| Daphnid | 48-h | LC50 | >100 | | " " |
| Green Algae | 96-h | EC50 | 8.4 | 280 | " " |
| Fish | - | Chronic Value | >10 | 78 | Est Top Left; Anlg [REDACTED] ACR10 |
| Daphnid | - | Chronic Value | >10 | 29 | Est Top Left; Anlg [REDACTED] ACR10 |
| Green Algae | - | Chronic Value | 2.8 | 97 | " " |
| Ecotox Value Predictions are based on QSARs for substituted ureas Comments: (ECOSAR V2.0); MW 239; Log Kow = 0.60 (M, for mixture); solid with an unknown MP (P); S = 35 mg/L (M, for mixture), Reacts; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO ₃ ; and TOC <2.0 mg/L. | | | | | |

Ecotox Factors

| Factors | Most Sensitive Endpoint | Assessment Factor | CoC | Comment |
|------------------------|-------------------------|-------------------|------|---------|
| Acute Aquatic (ppb): | | 4 | 2100 | Algae |
| Chronic Aquatic (ppb): | | 10 | 280 | Algae |

| Factors | Values | Comments |
|--------------------|---------------------------------------|----------|
| SARs: | Substituted Ureas | |
| SAR Class: | Substituted Ureas-Thiophosphoramidate | |
| TSCA NCC Category? | <input type="text" value="None"/> | |

Recommended Testing:

Ecotox Factors Environmental

Comments: Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (<https://www.epa.gov/tsc-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model>). Based on these estimated hazard values from ECOSAR, EPA concludes that this chemical substance has moderate environmental hazard.

- Substance does not fall within the TSCA New Chemicals Categories.
- ECOSAR chemical class of Substituted Ureas.
- Analog data were considered for [REDACTED]
- Moderate hazard based on acute and chronic concentrations of concerns of 2,100 ppb and 280 ppb, respectively.

Comments/Telephone

Log

| Artifact | Update/Upload Time |
|----------|--------------------|
|----------|--------------------|